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National Nuclear Security Administration
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Performance Study and Optimization of FIeCSALE using Tabular Equation of State

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Objective

Explore new numerical and computer science approaches to efficiently use EOSPAC within the context of FIeCSALE and reduce the cost of equation of state (EOS) table queries

Motivation

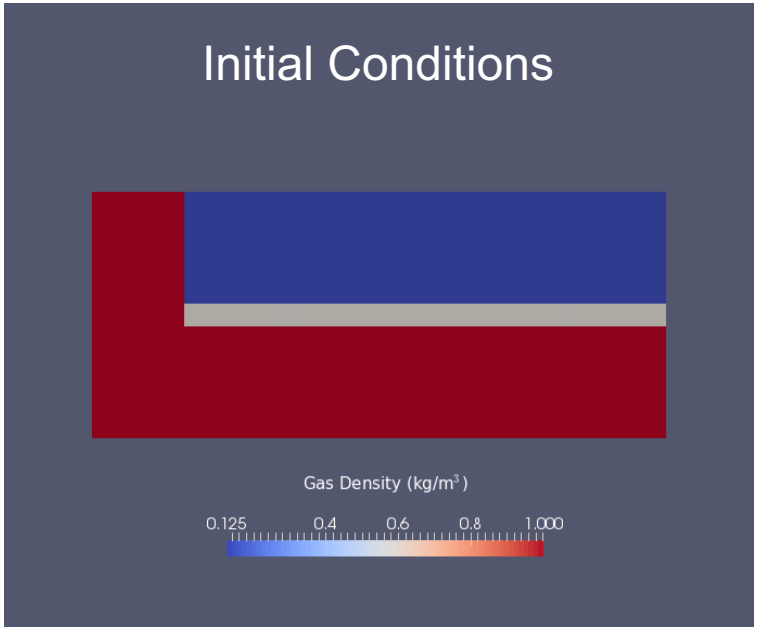
- Tabular equation of state (EOS) data are constantly queried by physics codes
- Queries can occur several times per time-step at each computational cell for each material that exists at a query location
- Queries regularly involve expensive interpolations of thermodynamic quantities
- Thermodynamic quantities are necessary for computation of additional physical quantities for the simulations
- Reducing the cost of tabular EOS queries provides an overall reduction in the solution time for many complex physics problems

FleCSALE, FleCSI, + EOSPAC

- **FleCSALE**
  - Continuum dynamics code, supports multi-phase fluids and tabular equation of state (EOS)
  - 2D/3D cell-centered Eulerian and Lagrangian solver
  - 3D FEM Lagrangian solver
- **FleCSI**
  - Compile-time configurable framework designed to support multi-physics application development
  - Supports an MPI and Legion backend
  - Primary structure is hierarchical, exposing low-level, mid-level, and high-level interfaces that are appropriate for different sets of users
- **EOSPAC**
  - Collection of interface routines
  - Used to access the SESAME data library
  - Can perform various data adjustments and interpolations on the SESAME data
  - Inherently serial execution

Triple Point Problem

- **Fluids simulation involving three different materials**
  - All materials are ideal gases
- **Problem decomposed into four regions**
  - Left-most and bottom regions: two different materials at the same density
  - Top region: third material at low density
  - Middle region: mixed composition & density
- **All materials can use tabular EOS data for the simulations.**



Bottlenecks and Strategies

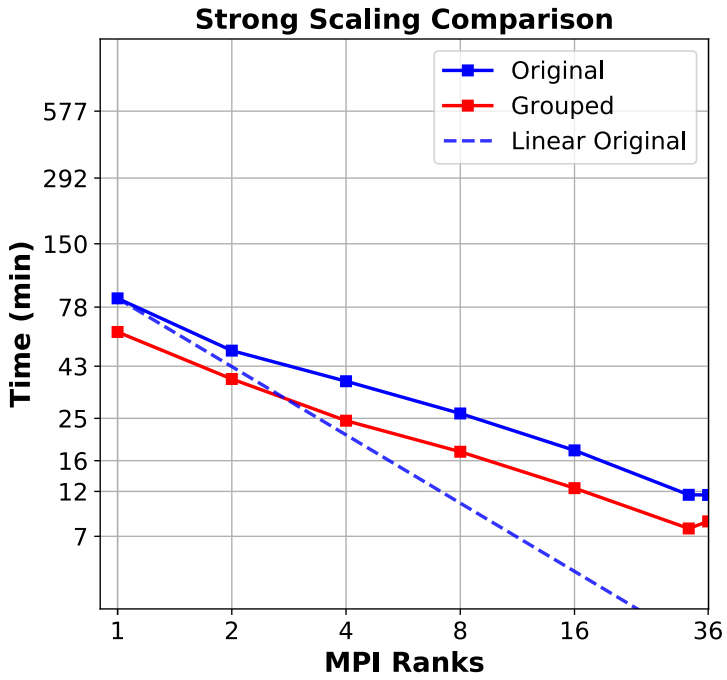
- **Initial Bottlenecks:**
  - Ghost Data Creation
  - Material Grouping
  - MPI Communication
  - Interpolation

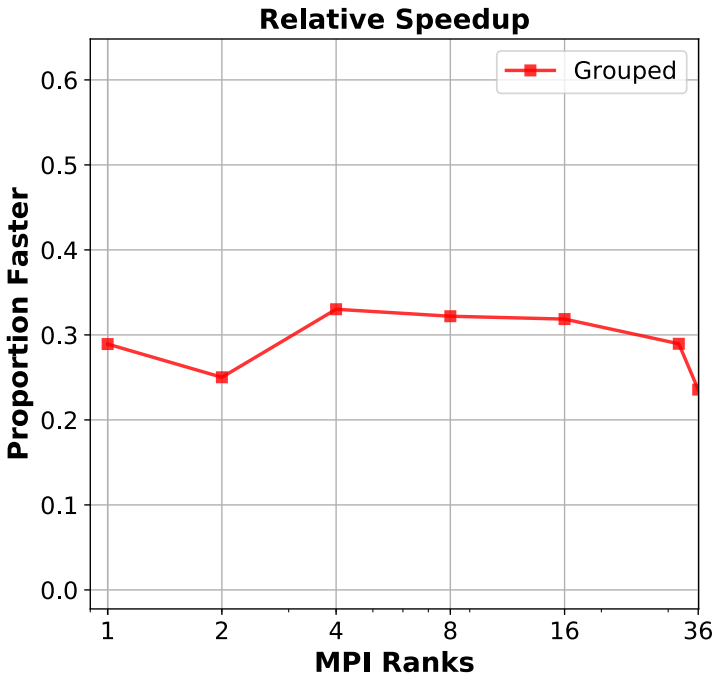
- **Explored Strategies:**
  - Software Engineering
  - MPI Communication Optimization --- sparse data
  - Hybrid Programming --- OpenMP
  - GPU Porting with different memory schemes
  - Machine Learning

Software Engineering

FleCSALE/EOSPAC Linking

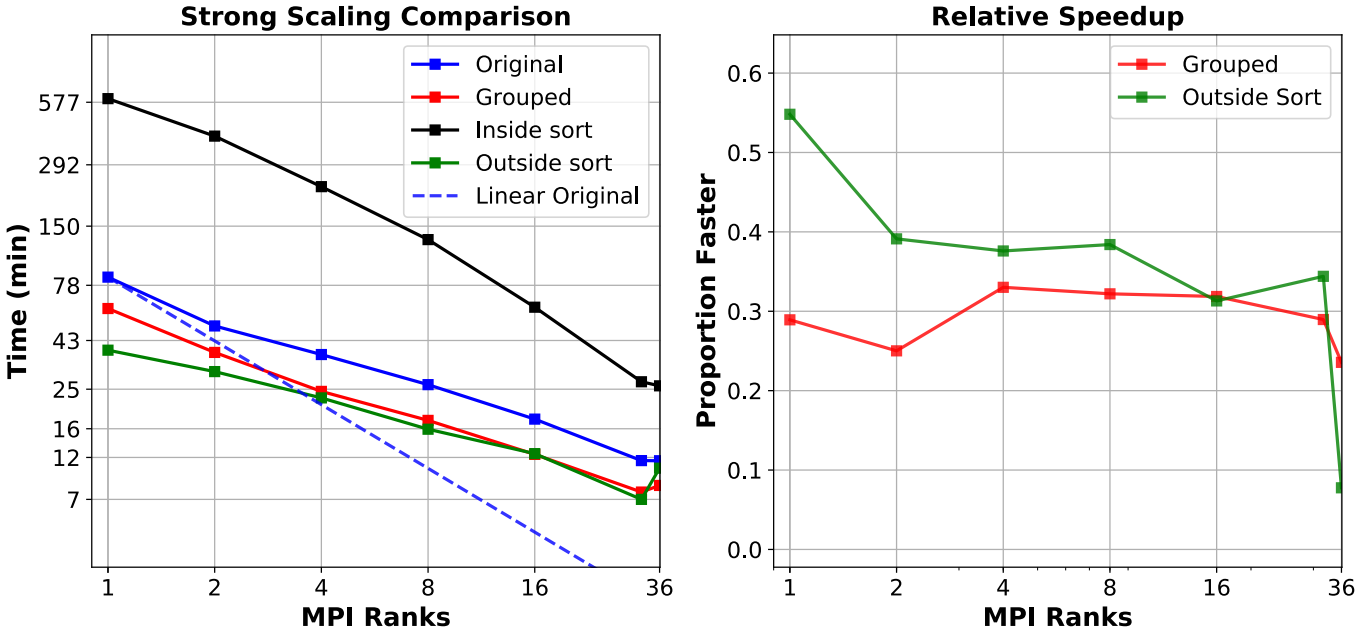
- Linking Optimizations:
  - Enabled the inversion/storing of modified Sesame tables at the initialization of FleCSALE
  - Reformatted FleCSALE to send common material cells to EOSPAC as groups





Sorting in EOSPAC's Search Algorithm

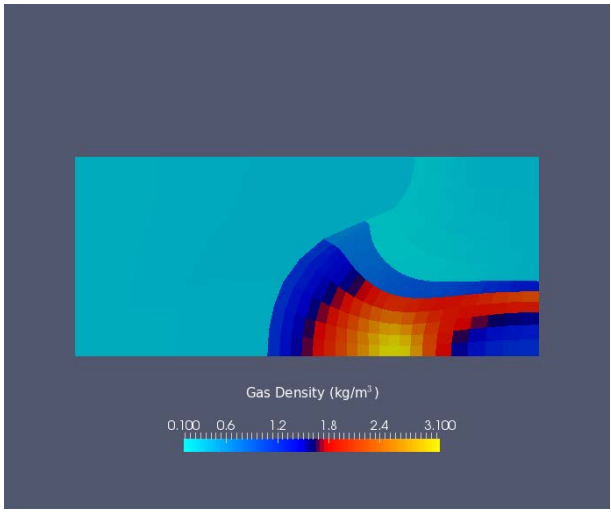
- Before interpolations, EOSPAC places a stencil on the material table → eos_srchdf()
- Approach uses an input to eos_srchdf() which gives the first point for the table sweep
- The indexes of the array of points to be interpolated are sorted before sweeping
- Two versions:
  - Embedded in EOSPAC
  - Inside of FleCSALE



Problem-Dependent Performance

- There is potential for enhanced performance from the index sorting which is problem dependent

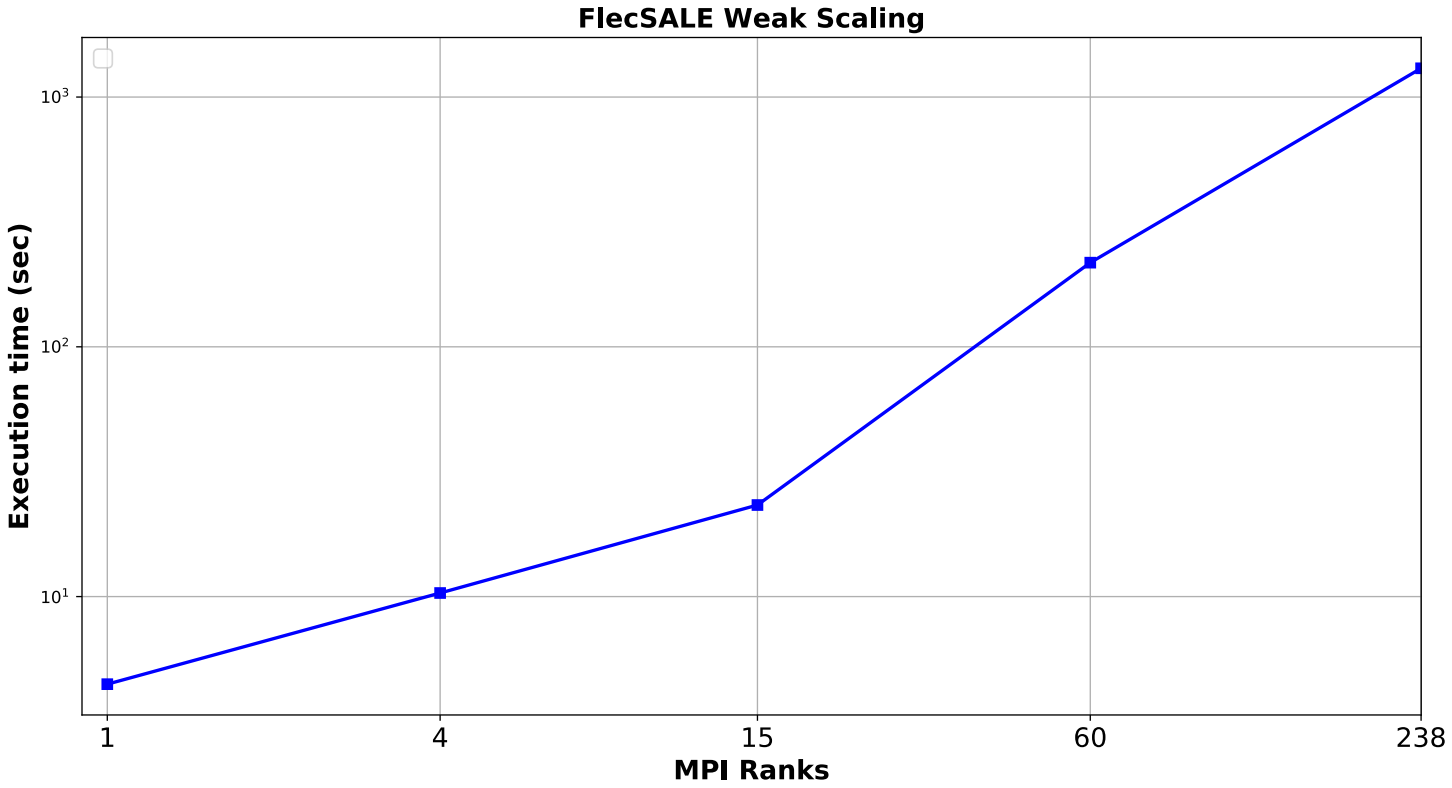
- Example: CDSS Scaling Problem (Triple Point)
  - Simulation density range = 0 to 3.5
  - Sesame table range = 0 to ~61,000
  - We only use roughly 20% of the table for this problem



- Problems with larger property variations are more likely to obtain better performance with the sorting approach

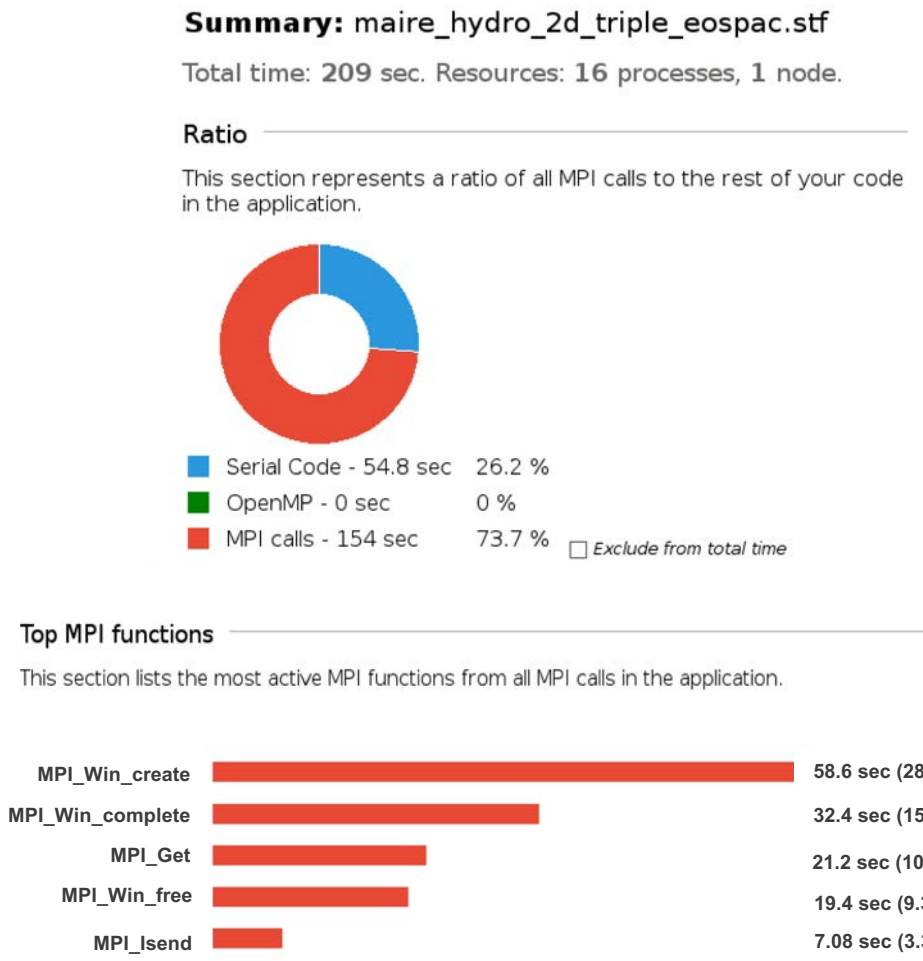
Sparse Data Optimization

Motivation


FlecSALE Weak Scaling
Execution time (sec)
10^3
10^2
10^1
1
4
15
60
238
MPI Ranks

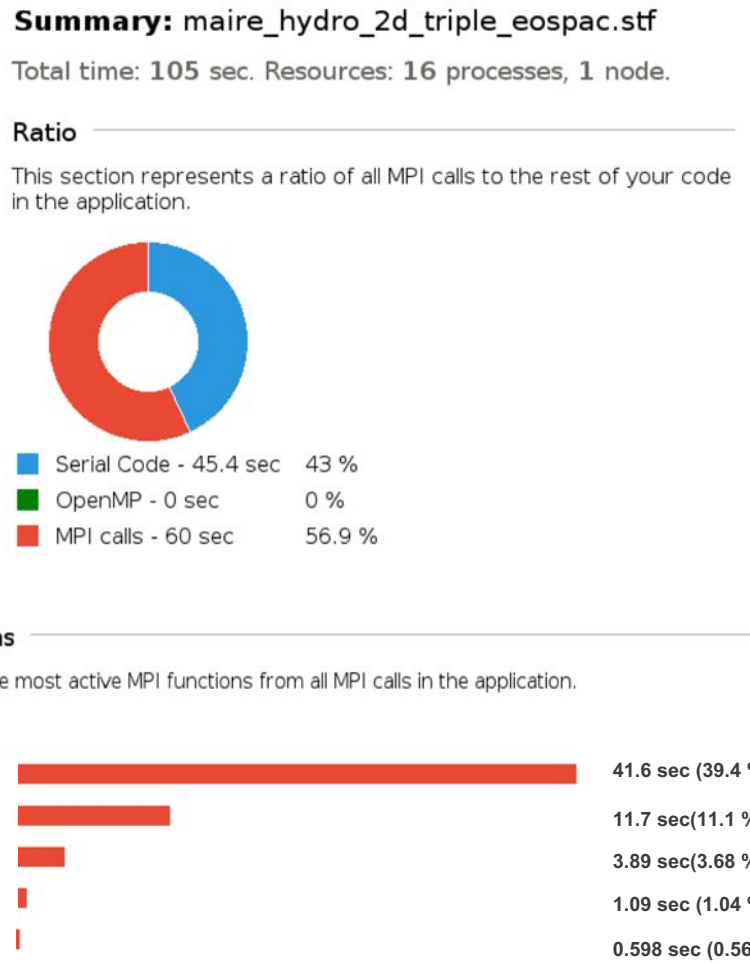
Sparse Data Optimization

- Weak scaling graph shows huge communication latency
- MPI backend in FleCSI uses One Sided Communication
- Tracing the application showed ~74% of the code was MPI communication calls
- **MPI_Win_create** calls was the most expensive with ~28% of the execution time



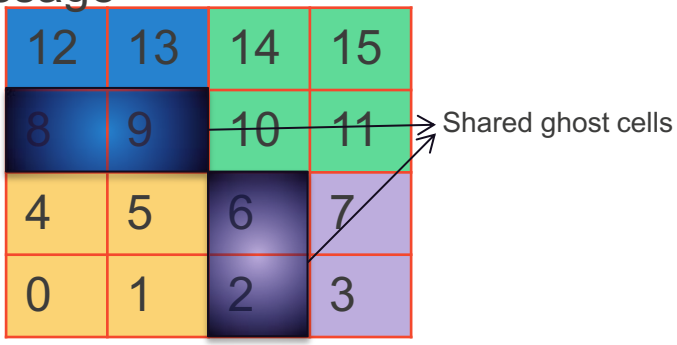
Sparse Data Optimization –Copy removal

- Unnecessary copies of data were eliminated
- Shared window creation was done only once with reduction of **MPI_Win_create** calls
- MPI Communications takes about ~57%
- **Performance Improvement**
  - Single node ~20%
  - Multi node ~40%



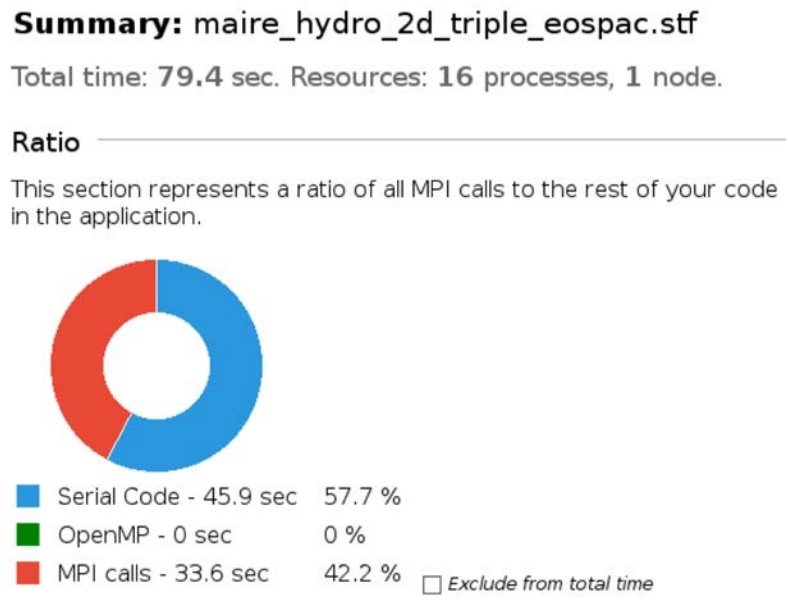
Sparse Data Optimization- MPI_Datatype

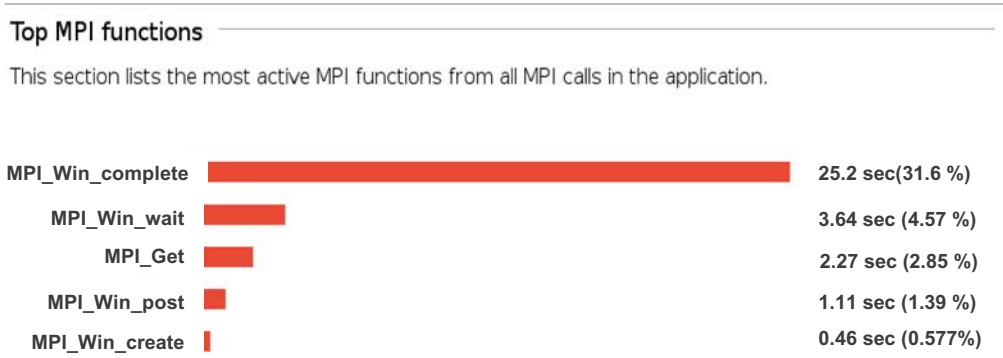
- **MPI_Datatype** is used for shared ghost cells to treat as a single message



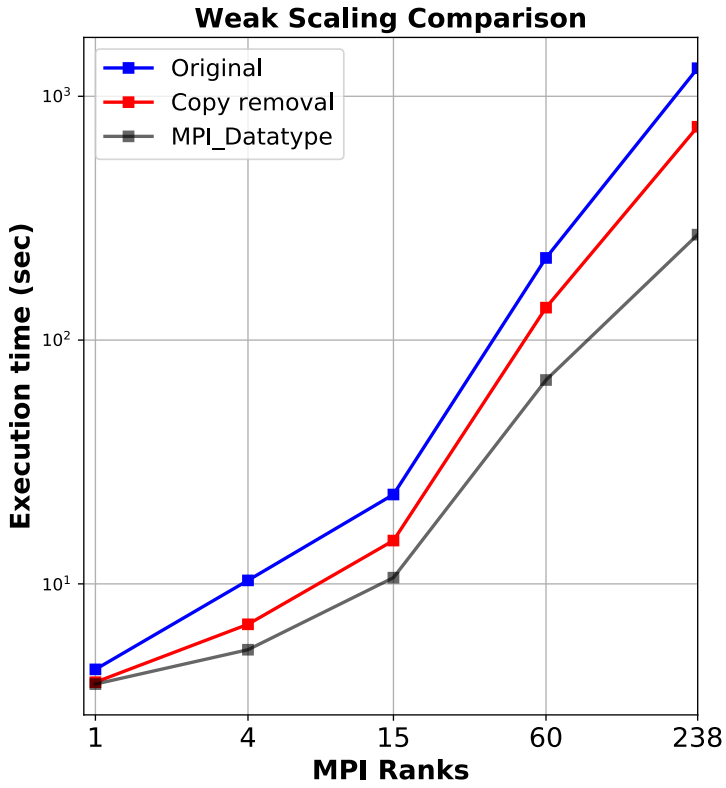
- **MPI_Get** and **MPI_Win_complete** calls reduced
- MPI Communication takes about 43%

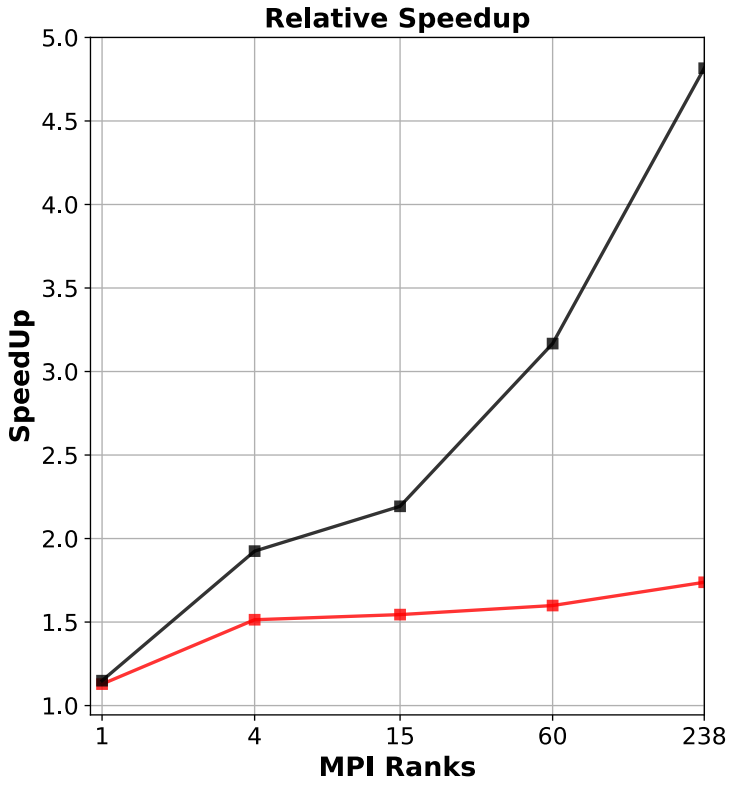
- **Performance Improvement**
  - Single node ~25%
  - Multi node ~60%





Performance Analysis



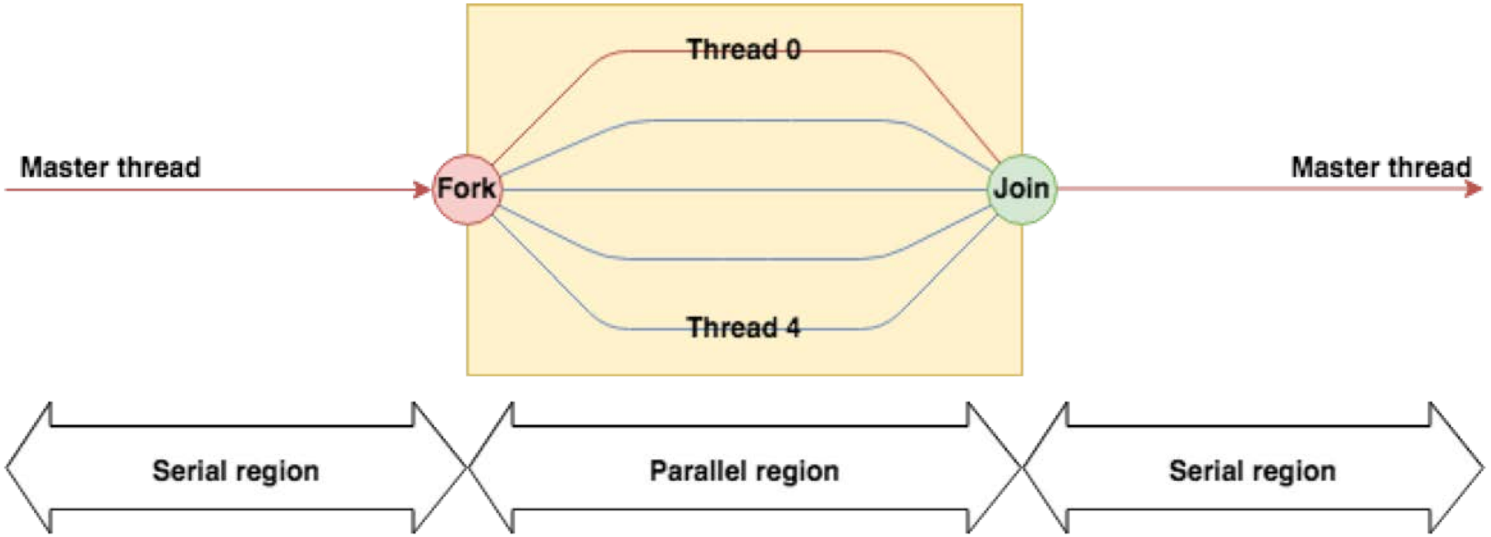


- Overall performance improvement ~80%
- Speedup of ~5x
- MPI_Win_complete is still expensive

Hybrid programming with OpenMP

Adding OpenMP in FleCSALE

- **Fork/join model:**

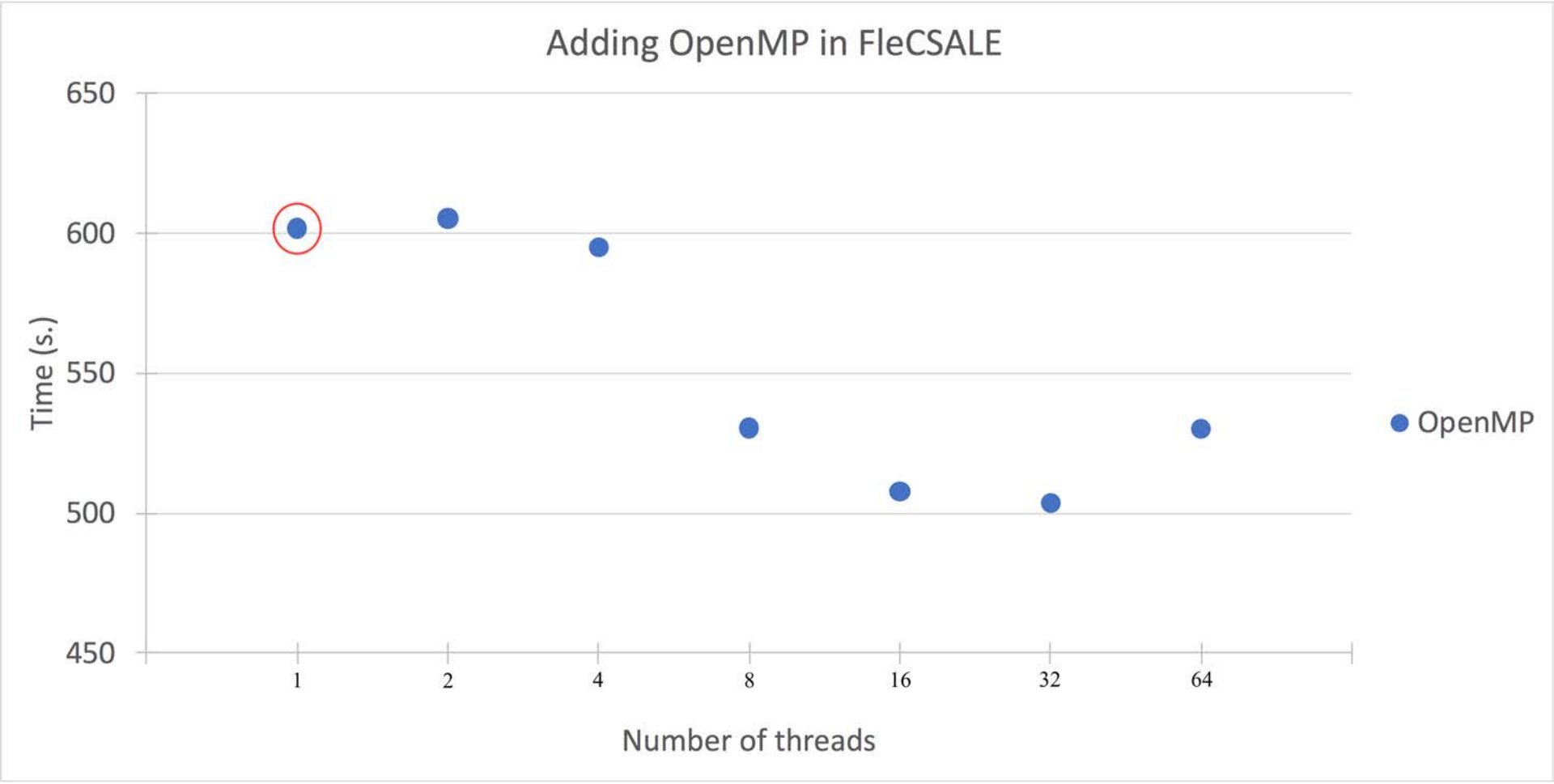


- **Two OpenMP approaches were investigated:**
  - tasking;
  - for-loop work-sharing.

Adding OpenMP in Flecsale

- **Changes done in:** maire_hydro/tasks.h
- **Mesh:** triple_200x81.g
- **Flags:** -g -O3 -fopenmp
- **Compilers:** gcc/7.3.0 and intel/18.0.2
- **MPI implementation:** mpich/3.2.1-intel_18.0.2
- **Platform:** Intel Haswell --- E5-2698 v3
  - Sockets --- 2
  - Cores per Socket --- 16
  - NUMA Domains --- 2

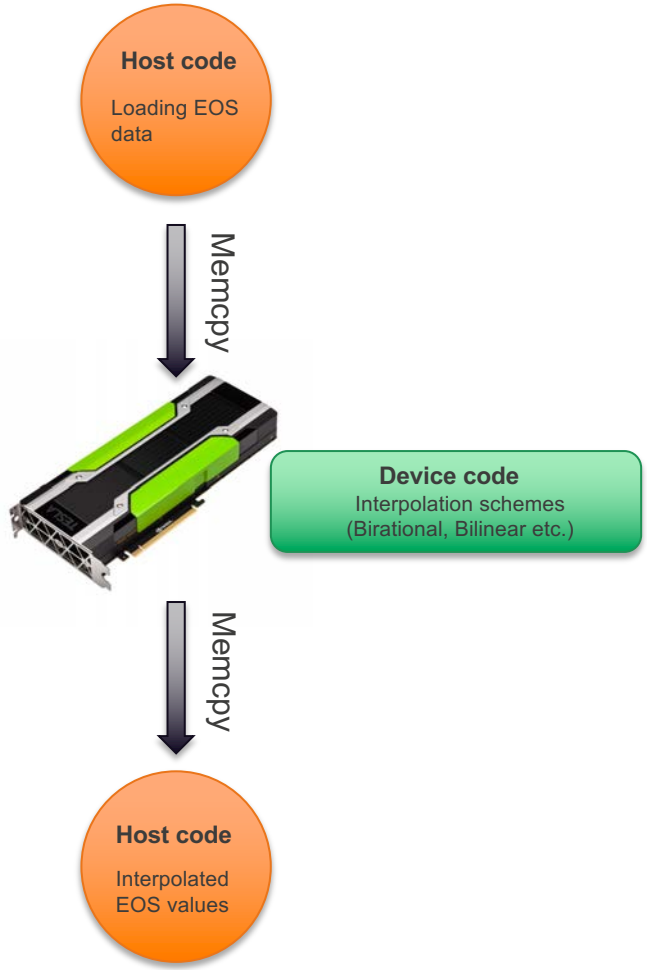
Performance results



GPU Porting for EOSPAC

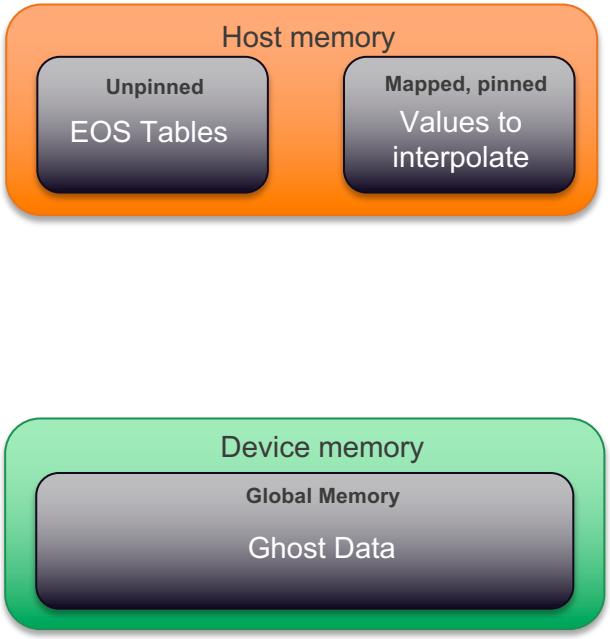
Motivation

- FleCSALE queries EOSPAC for interpolated EOS values.
- Profiling revealed Interpolation was costliest part of FleCSALE, ~15% of simulation.
- Can be parallelized easily.
- GPUs are next generation hardware for intensive computations.
- Interpolation is not memory intensive.



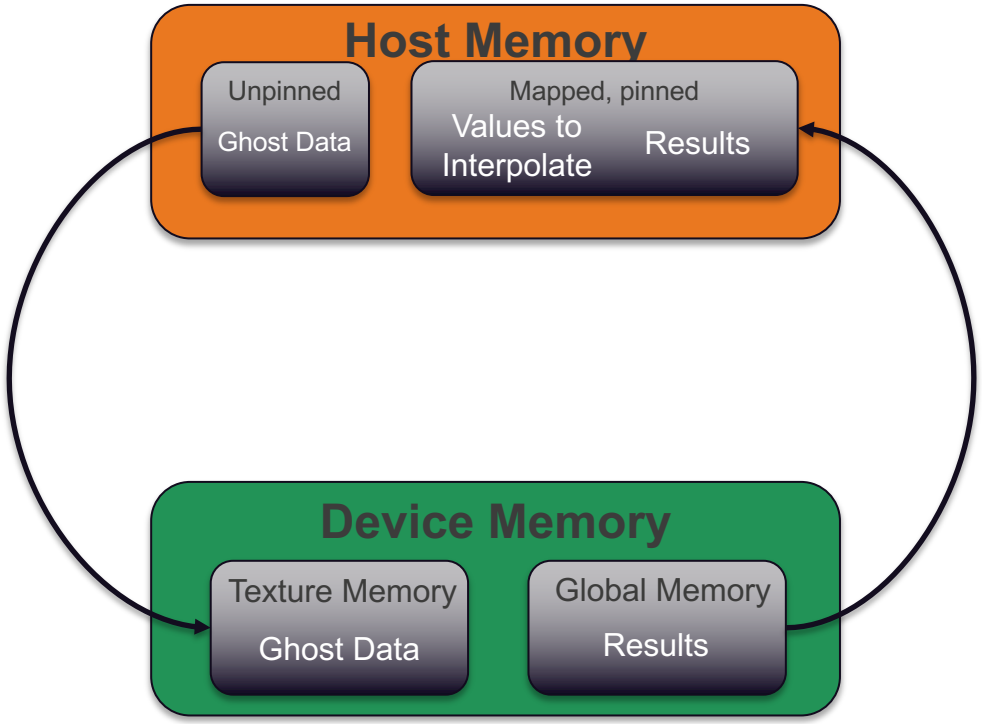
Methodology

- Wrapper around Birational Interpolation kernel and Bilinear Interpolation kernel that can be called inside EOSPAC.
- No changes to the public interfaces. Only need a separate library compilation.
- Interpolation algorithms are called multiple times within a single FleCSALE time-step.
- No Memcpy is necessary for the interpolated values.

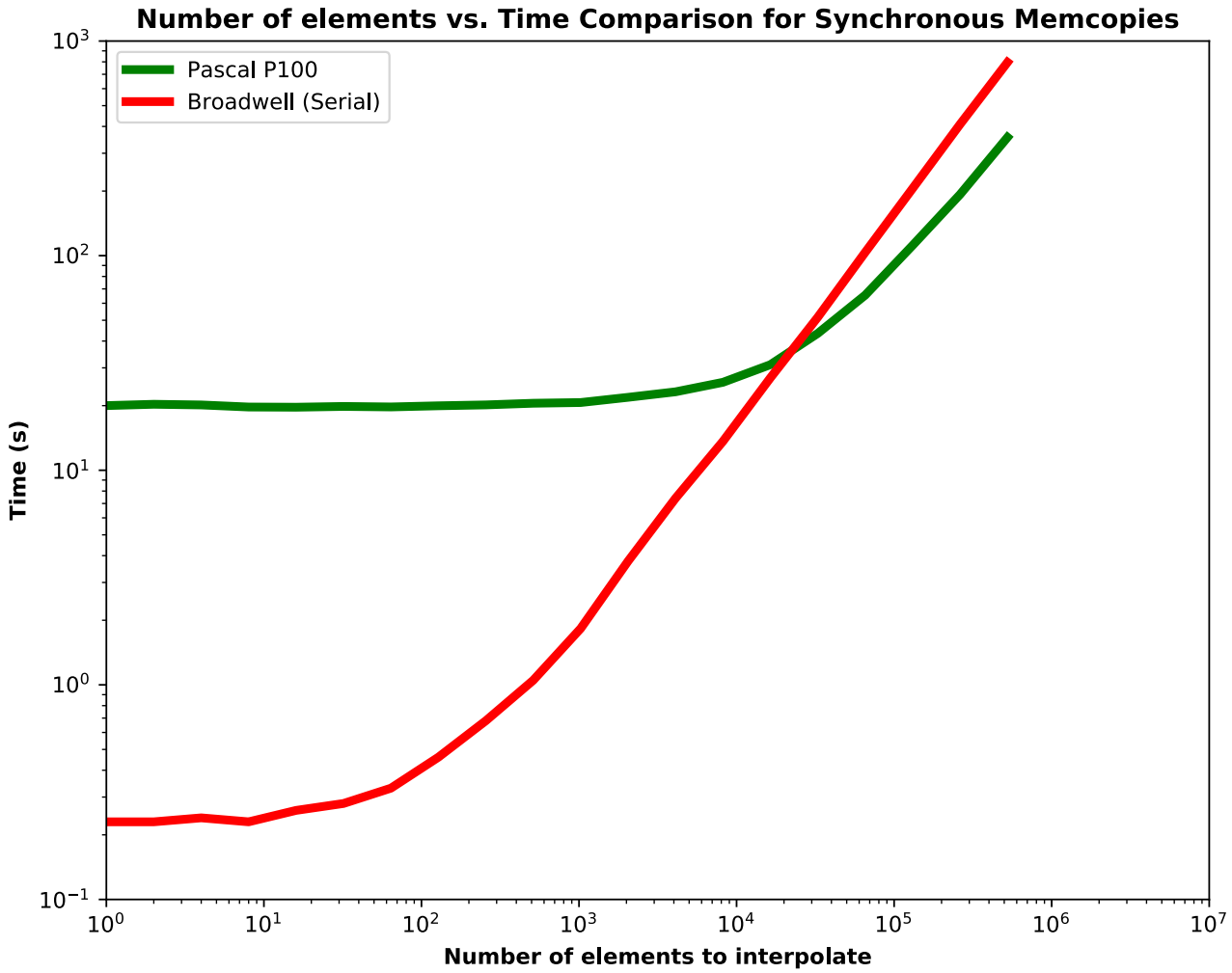


Bilinear Interpolation

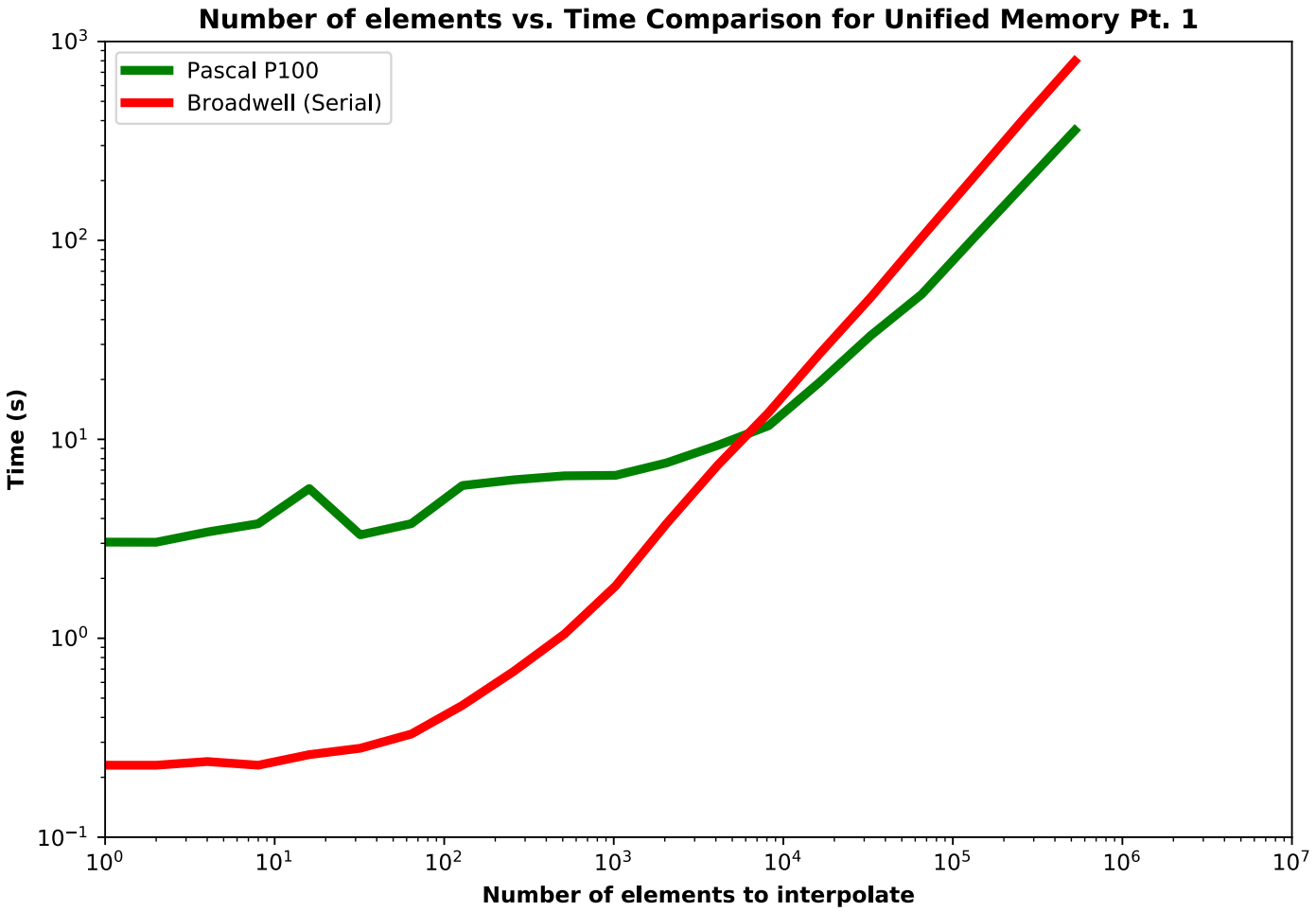
- Can be executed by the hardware using texture memory.
- Requires the use of 32 bit, single precision data types
- Use of single precision types provides an improved processing throughput of at least 2x, depending on architecture
- Texture memory allows us to store tables in the unified L1 cache/texture cache



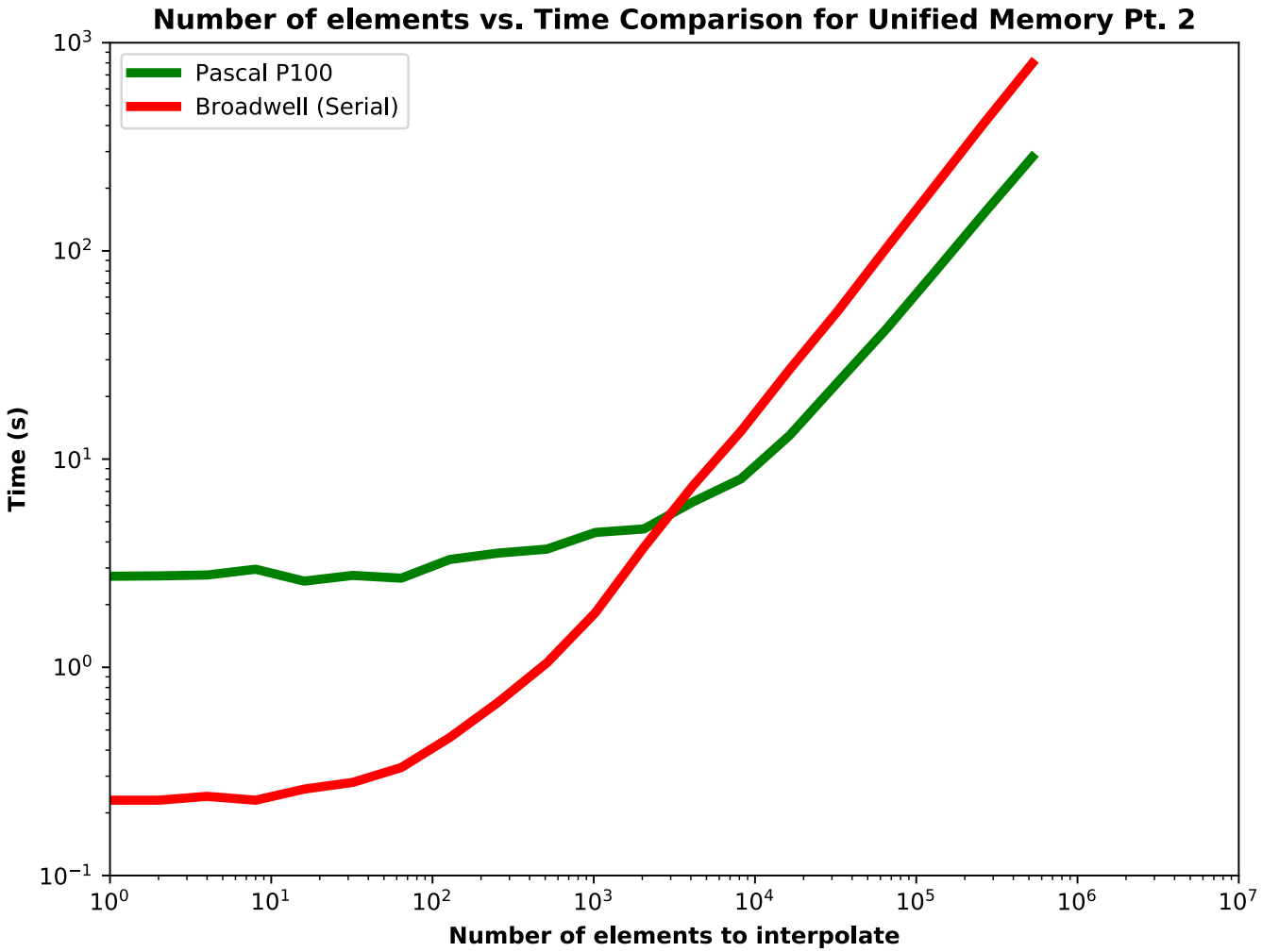
Speed-up from CUDA



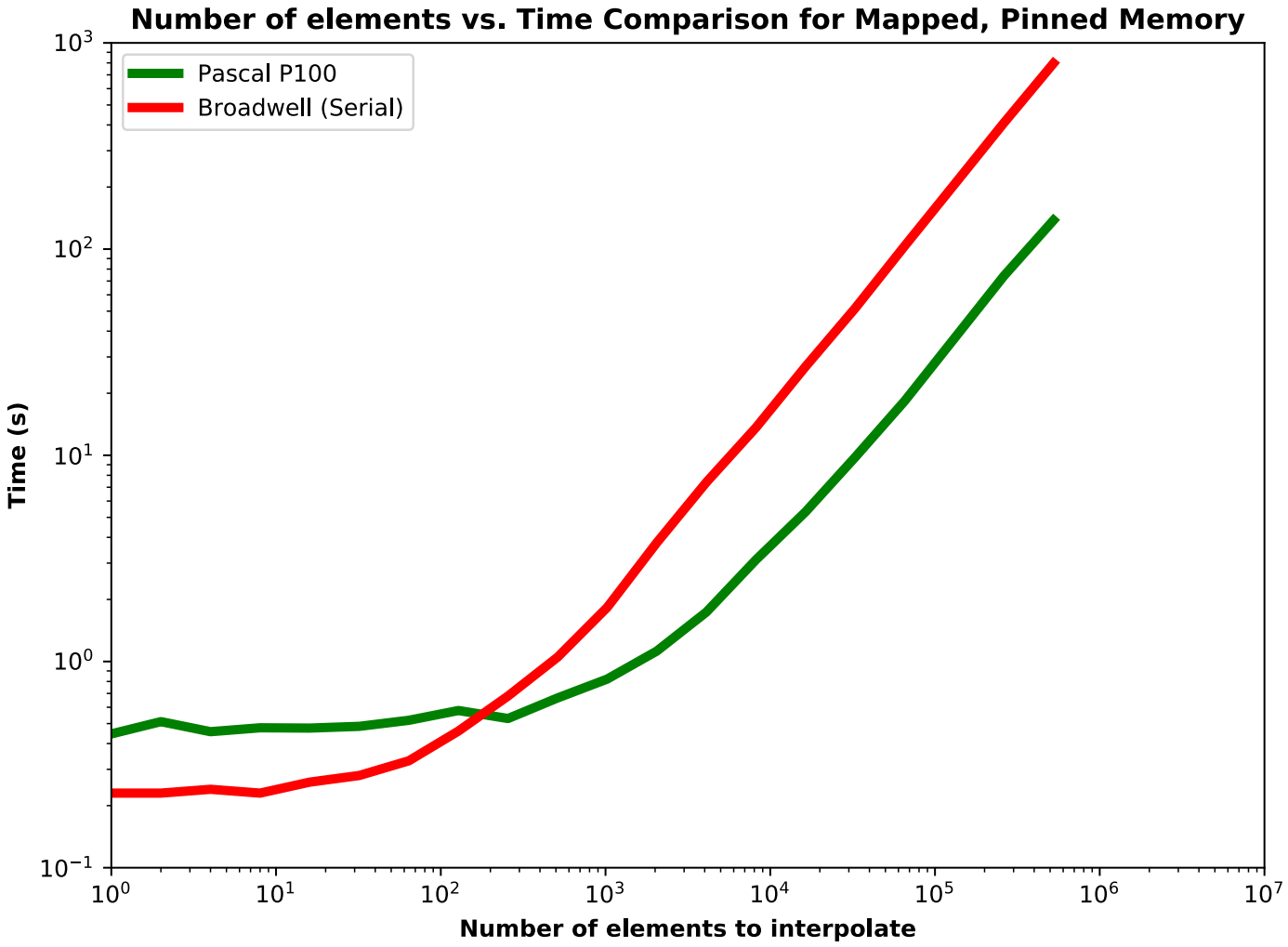
Speed-up from CUDA



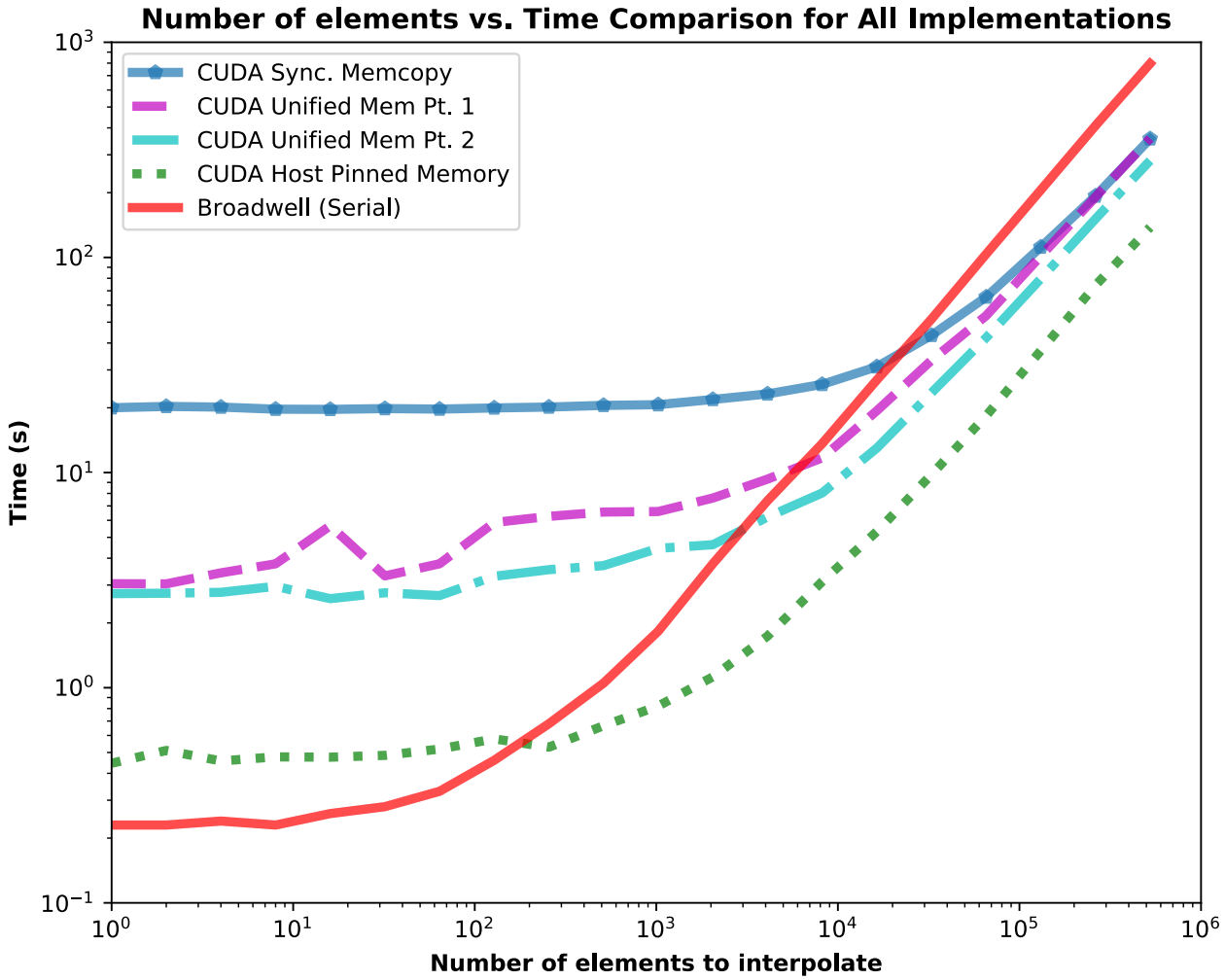
Speed-up from CUDA



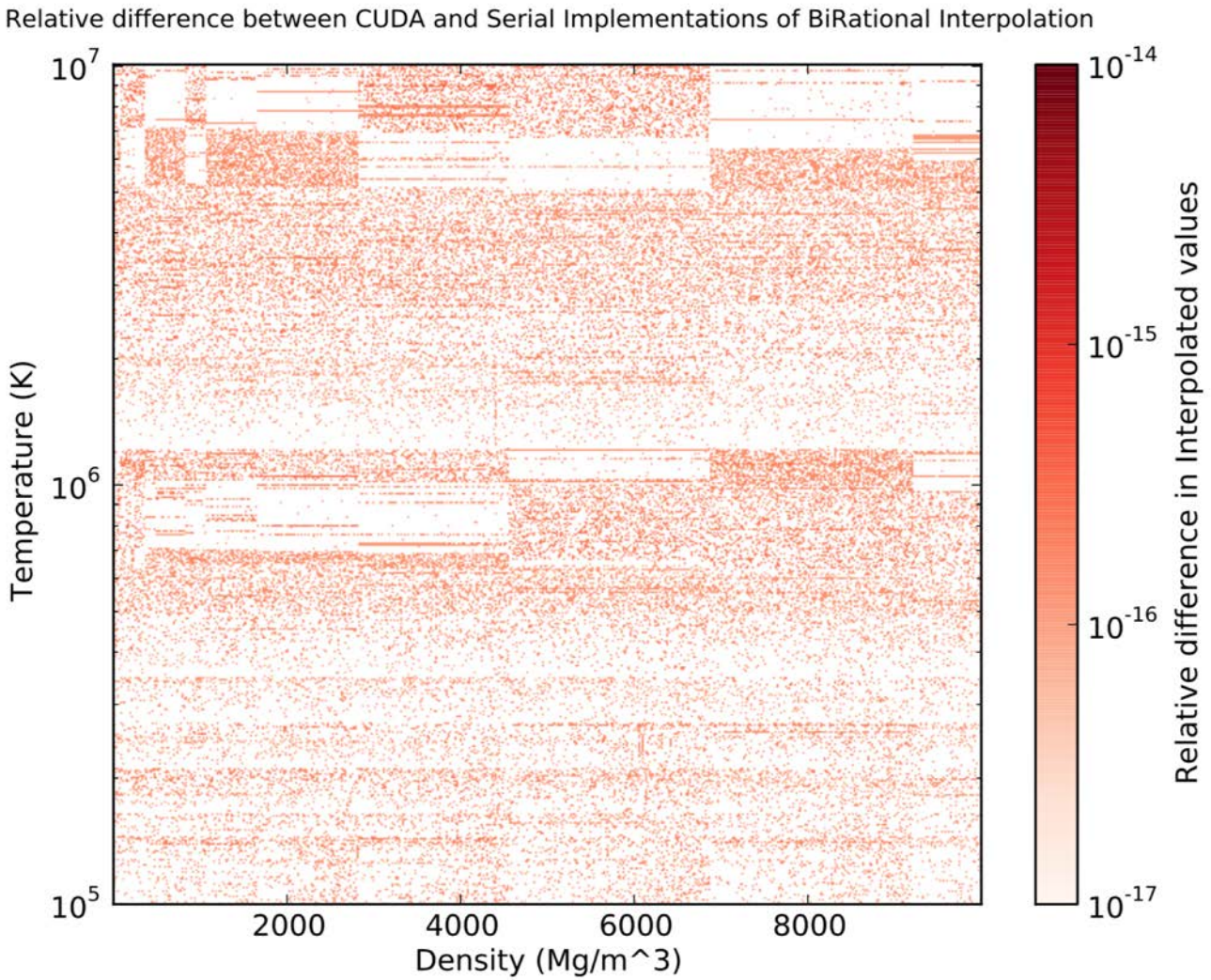
Speed-up from CUDA



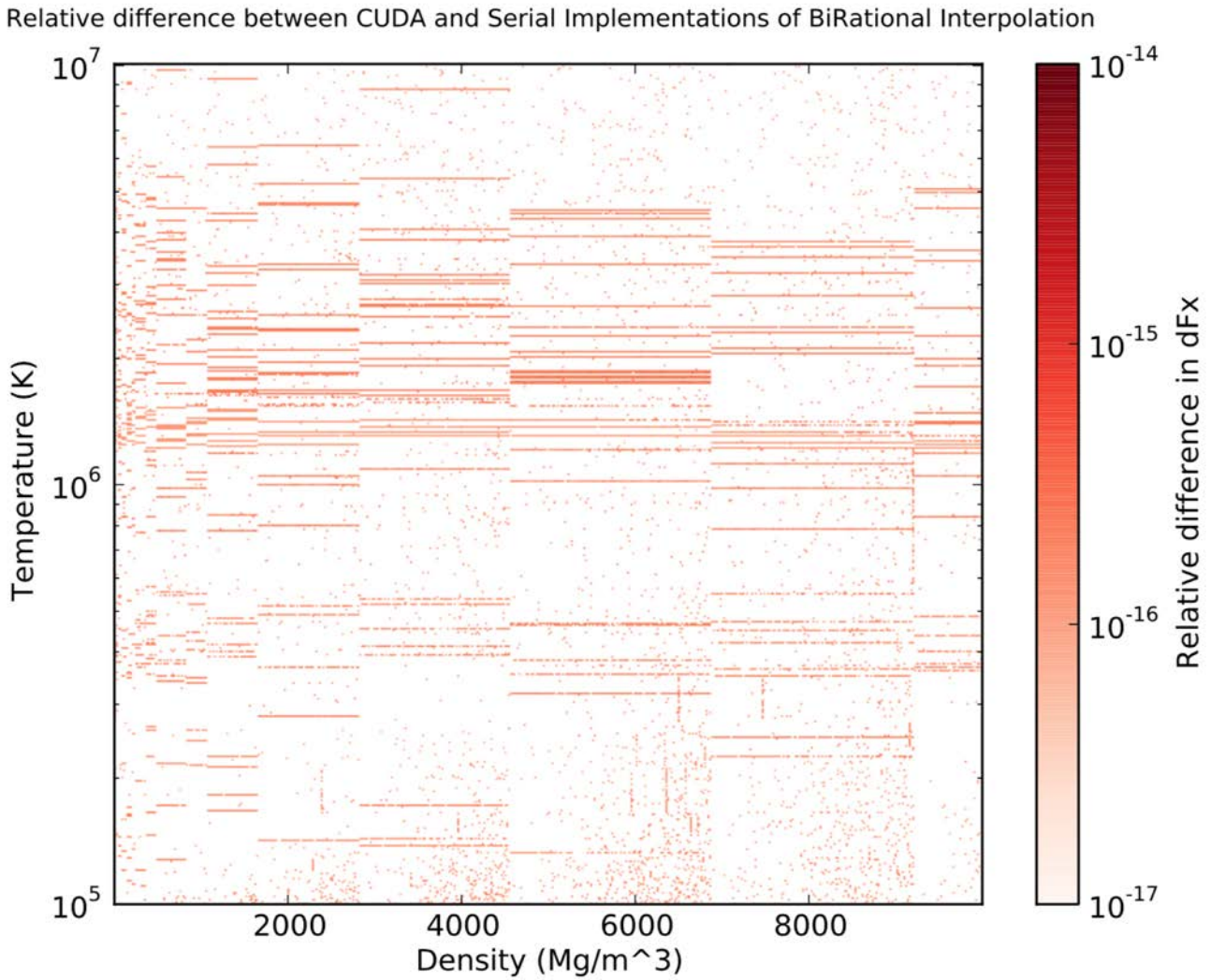
Speed-up from CUDA



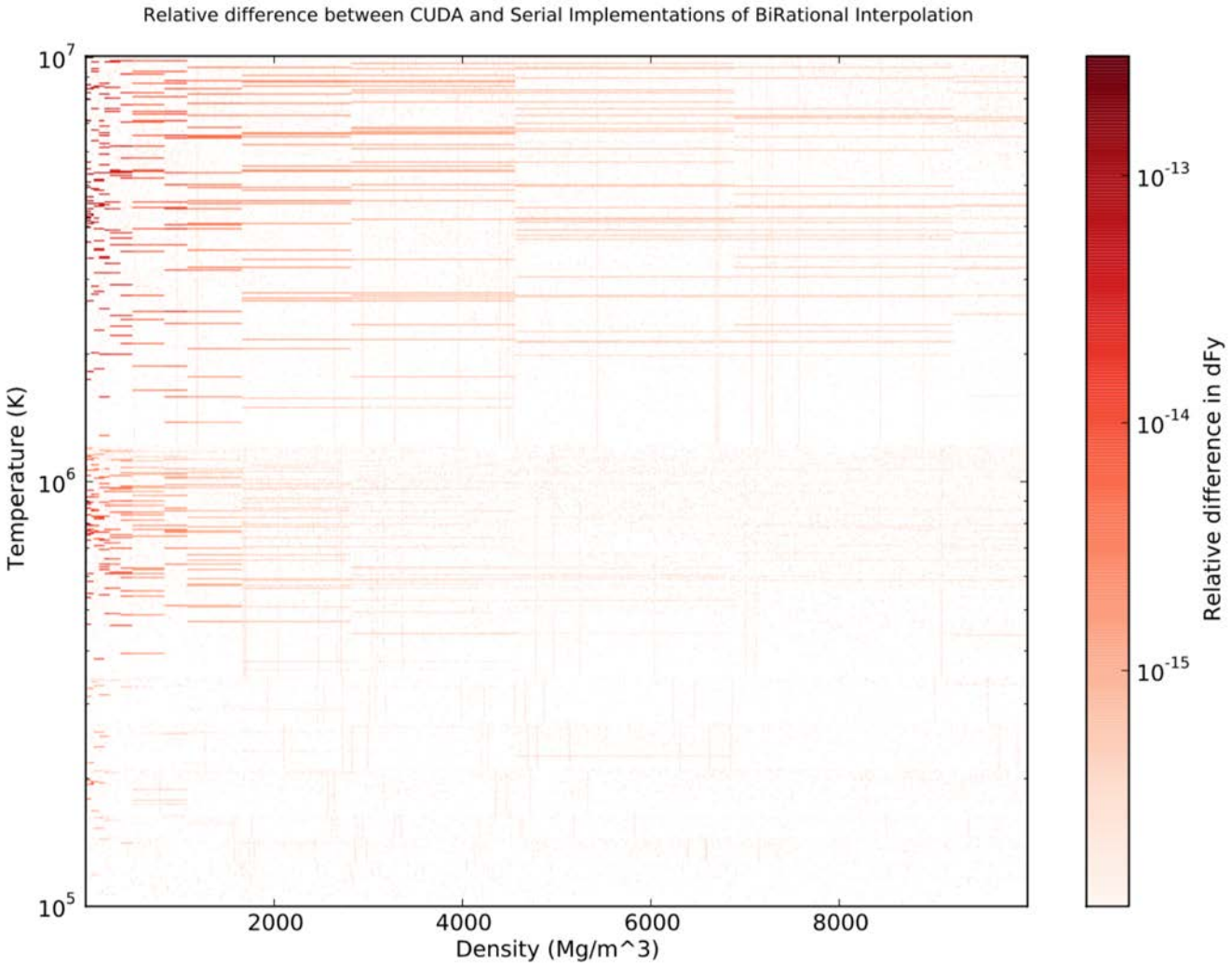
Accuracy for Sesame 3720



Accuracy for Sesame 3720



Accuracy for Sesame 3720



Machine Learning for EOS Interpolation

Machine Learning for EOS Interpolation

Goal: Replace calls to EOSPAC with ML regression.

Process:

1. Generate a training dataset using EOSPAC
2. Train the model
3. Characterize the error (compared to EOSPAC)
4. Integrate with FleCSALE

ML Models:

- Kernel Ridge Regression (KRR)
- Random Forest (RF)

Model Framework

Nomenclature: density (d), internal energy (ie), pressure (p), temperature (T), soundspeed (ss)

Pressure model

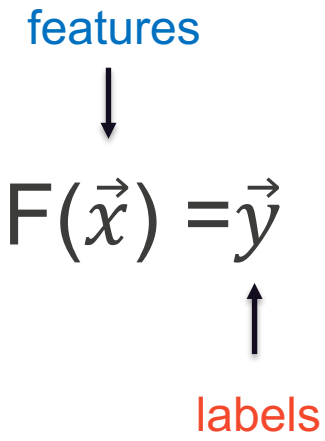
- F(d,ie) = p

Temperature model

- F(d,ie,p)=T

Soundspeed model

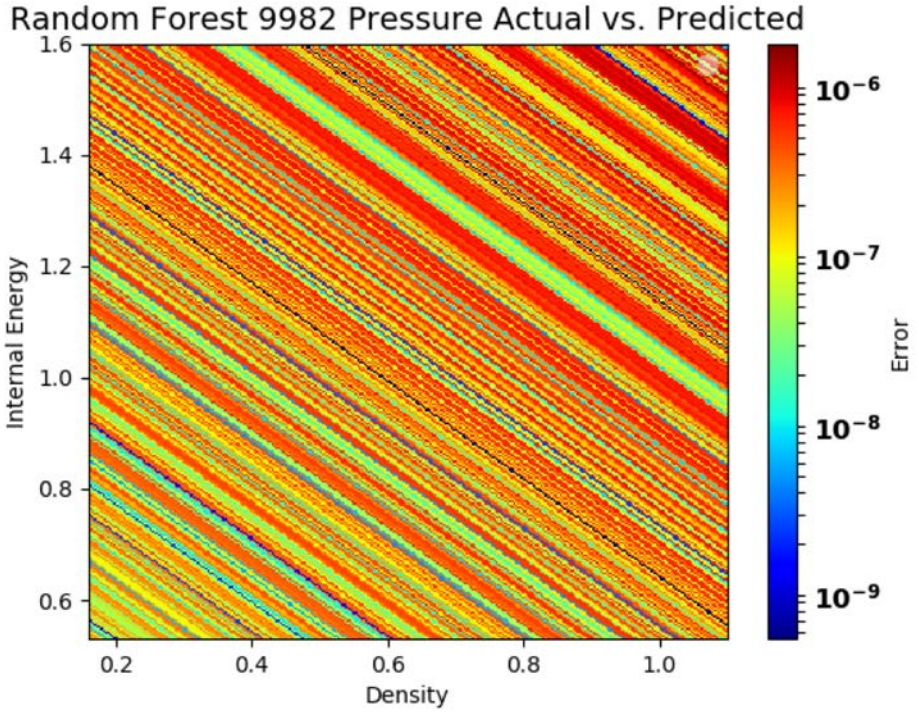
- F(d,ie,p,T) = ss

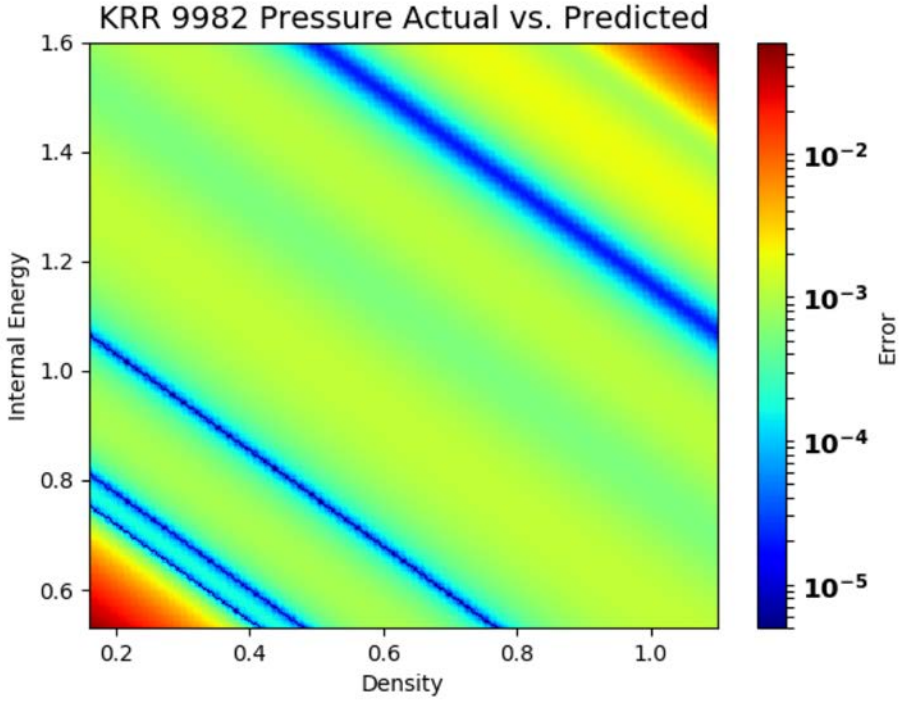


Machine Learning Error Analysis

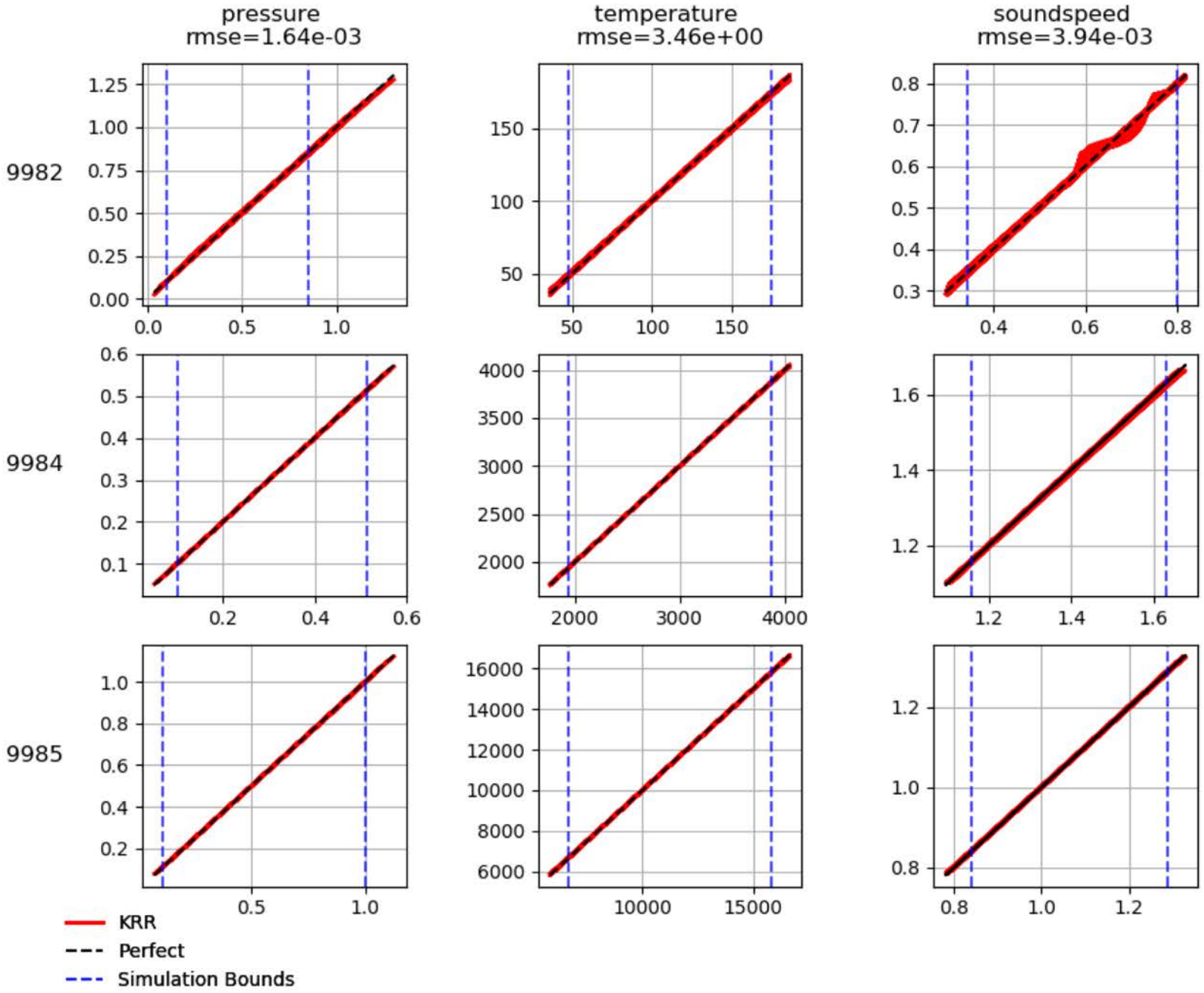
Random forest vs. Kernel Ridge Regression

- RF is more accurate but much slower
- RF takes ~3GB
- KRR takes ~1.5KB

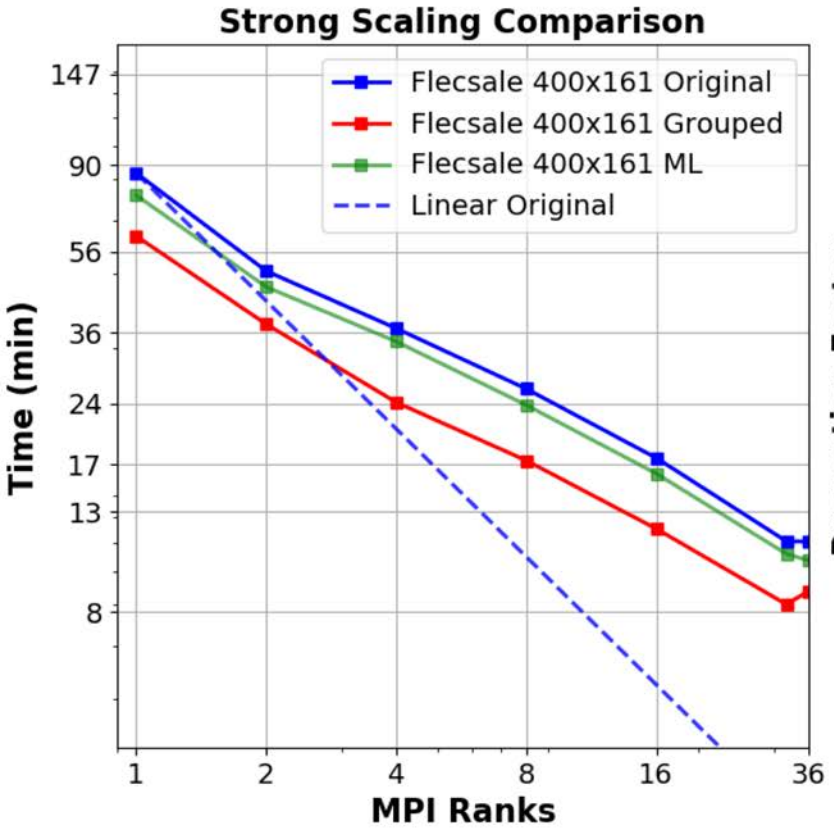


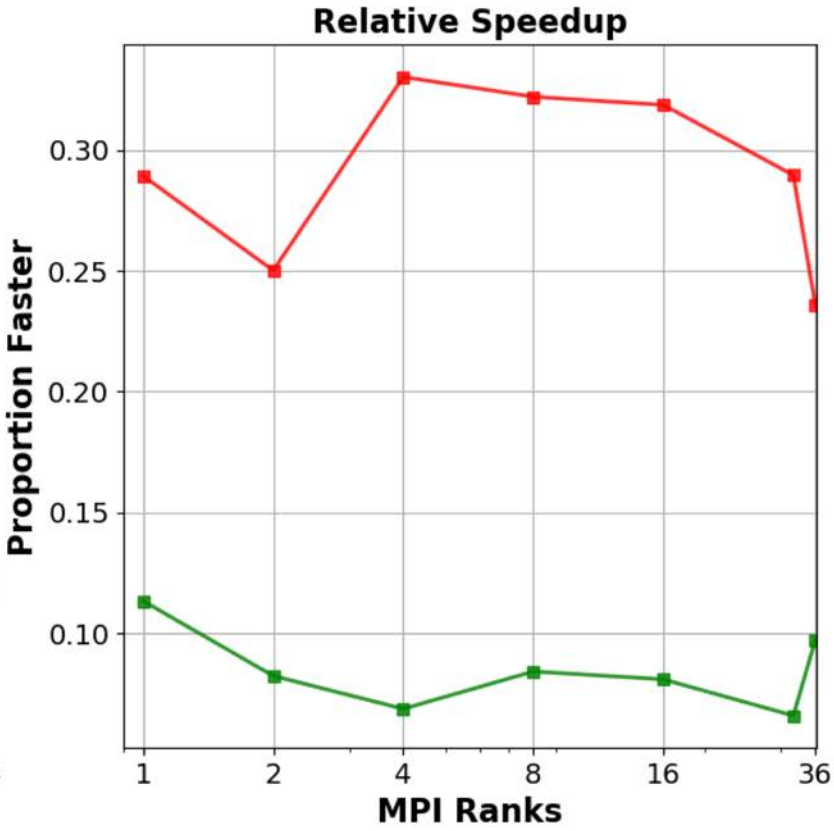


KRR Correlation plots



On-node Performance Comparison





Machine Learning Take-aways

- Accuracy and speed tradeoff
- Even with low accuracy, performance is questionable (in this case)
- Other ML models and C++ libraries exist

Final Results

Results

- **Proper selection of integration options and algorithms within EOSPAC provide a noticeable speed-up in FleCSALE**
- **Sparse data optimization with MPI backend shows a significant improvement about ~5x speed-up**
- **Initial CUDA results are promising and show a considerable speedup. However, integration with FleCSALE and host code optimizations are still required**
- **Initial machine learning integration did not increase performance, but other models and libraries could offer improvements**

Future Pursuits

- Add additional host code optimizations that allow for additional GPU performance improvements
- Take advantage of additional memory management schemes to further reduce the memory latency involved with GPU usage
- Study the performance of MPI and Legion backends, with and without the additional optimizations
- Utilize different parallel programming models within FleCSALE, (e.g., MPI + CUDA)
- Explore other types of Target Synchronization techniques for MPI communication like MPI_Lock, MPI_Unlock.
- Investigate other machine learning libraries (e.g., TensorFlow, MLPACK)

Acknowledgements

Thank you to the Co-Design Mentors, FleCSI Development Team, CCS-7, ISTI, ASC, & LANL